ROYAL SOCIETY OF CHEMISTRY | CHEMICAL INFORMATION AND COMPUTER APPLICATIONS GROUP

NEWSLETTER summer 2017

Above: Members of the RSC CICAG Committee meet at Burlington House this May

CICAG aims to keep its members abreast of the latest activities, services, and developments in all aspects of chemical information, from generation through to archiving, and in the computer applications used in this rapidly changing area through meetings, newsletters and professional networking.

Chemical Information & Computer Applications Group Websites:
http://www.rsc.org/CICAG
https://www.liverpool.ac.uk/~ngberry/cicag/index.htm

LinkedIn http://www.linkedin.com/groups?gid=1989945

MyRSC http://my.rsc.org/groups/cicag

https://twitter.com/RSC_CICAG

QR Code

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Stuart Newbold, email: stuart@psandim.com

Chemical Information & Computer Applications Group Chair's Report

Contributed by RSC CICAG Chair Dr Helen Cooke, email: helen.cooke100@gmail.com

This is my final Chair's report, as after three years I have come to the end of my term of office. I am delighted that CICAG Committee member Chris Swain, Director and Founder of Cambridge MedChem Consulting, has taken over the role.

Another change is that Stephanie North decided to resign from the Committee in February. Many thanks to Stephanie, who joined the Committee in 2011, for her many contributions, including her regular Newsletter articles and acting as a judge on the RSC's Undergraduate Research Bursary Panel in 2016 (this role has been taken over by Neil Berry).

The first half of 2017 has been a busy period for CICAG's Committee. Here are a few highlights, all of which have more in-depth articles later in this newsletter:

- On 22 June, we held a scientific meeting at the University of Liverpool, Chemical Structure Representation: what would Dalton do now? We were pleased to be able to sponsor a student bursary, enabling Gianmarco Ghiandoni, a first year PhD student in the Information School at the University of Sheffield, to attend. We are grateful to the CSA Trust for sponsorship of keynote speaker Evan Bolton's expenses.
- We will again be sponsoring an Undergraduate Research Bursary over the summer. The successful applicant is Grzegorz Winter, a student in the School of Chemistry at Newcastle University.
- We are working with the Historical Interest Group and the RSC's Library to help promote the use of the RSC's digitised collection and have developed guidance notes for its access and use. We also intend to run some training webinars later in the year.
- A number of exciting meetings are being planned, most being organised in partnership with other RSC interest groups or external organisations.

Finally, I would like to thank all Committee members for their support and inspiration during my term as Chair. We have an excellent team with a diversity of experience and interests and I have enjoyed working with them all to further the aims of CICAG. I will be continuing as an ordinary Committee member, and am also a member of the North Staffordshire Local Section Committee. My remaining spare time will be taken up with voluntary work at Nantwich Museum, where I am a member of the Research Group and have recently been elected as a Trustee and Director.

Thank You, Helen Cooke

Contributed by RSC CICAG Newsletter Editor Stuart Newbold, email: stuart@psandim.com

A big thank you to Dr Helen Cooke, who has stepped down as CICAG Committee Chair, a role Helen took on when joining the group in in the summer of 2014. The Committee thanks Helen for the invaluable role she has played in steering the Committee over the last three years, overseeing numerous successful meetings and contributing greatly through liaison and organisation between groups both in and outside the RSC as well as communicating with RSC membership and support staff. CICAG is extremely pleased that Helen remains on the Committee.

An Introduction to CICAC New Chair, Chris Swain

Prior to founding Cambridge MedChem Consulting in 2006 Chris spent 20 years at Merck where he was formerly a Senior Director responsible for a medicinal chemistry and computational chemistry research group. At Merck he was the chemistry director for the project team that discovered and developed the NK1 antagonist Emend, work recognised with the RSC Biological and Medicinal Chemistry Sector award.

Chris current activities include providing collaborative medicinal chemistry and computational chemistry support to several small and mid-cap sized Pharma companies, biotech, academic groups, and to a number of projects supported by the Wellcome Trusts "Seeding Drug Discovery Initiative". He also acts as Chemistry Project Director for a Wellcome Trust funded research projects; he is a member of the Scientific Advisory Board of Selcia Ltd, and part of the Drug Discovery Advisory Group for Cancer Research UK. Chris works with the European Lead Factory as an Honest Data Broker providing advice and support to a number of project teams.

Chris has over 100 publications and is a named inventor on a similar number of patents. He has been an invited speaker at many international meetings and a regular contributor to various Medicinal chemistry courses and summer schools. He is a regular participant in the Cambridge Cheminformatics Network group, speaking on open source computational tools for drug discovery, and presenting at the Global health compound design webinars on "Using Jupyter as an electronic notebook to store and share computational chemistry".

As a member of the CICAG Chris has helped organise two meetings, the "Mobile Chemistry" meeting in Cambridge and "Cheminformatics for Drug Design: Data, Models and Tools" at Duxford. CICAG is extremely grateful to have Chris's wisdom and expertise on board as our new Chair.

CICAG Planned and Proposed Future Meetings

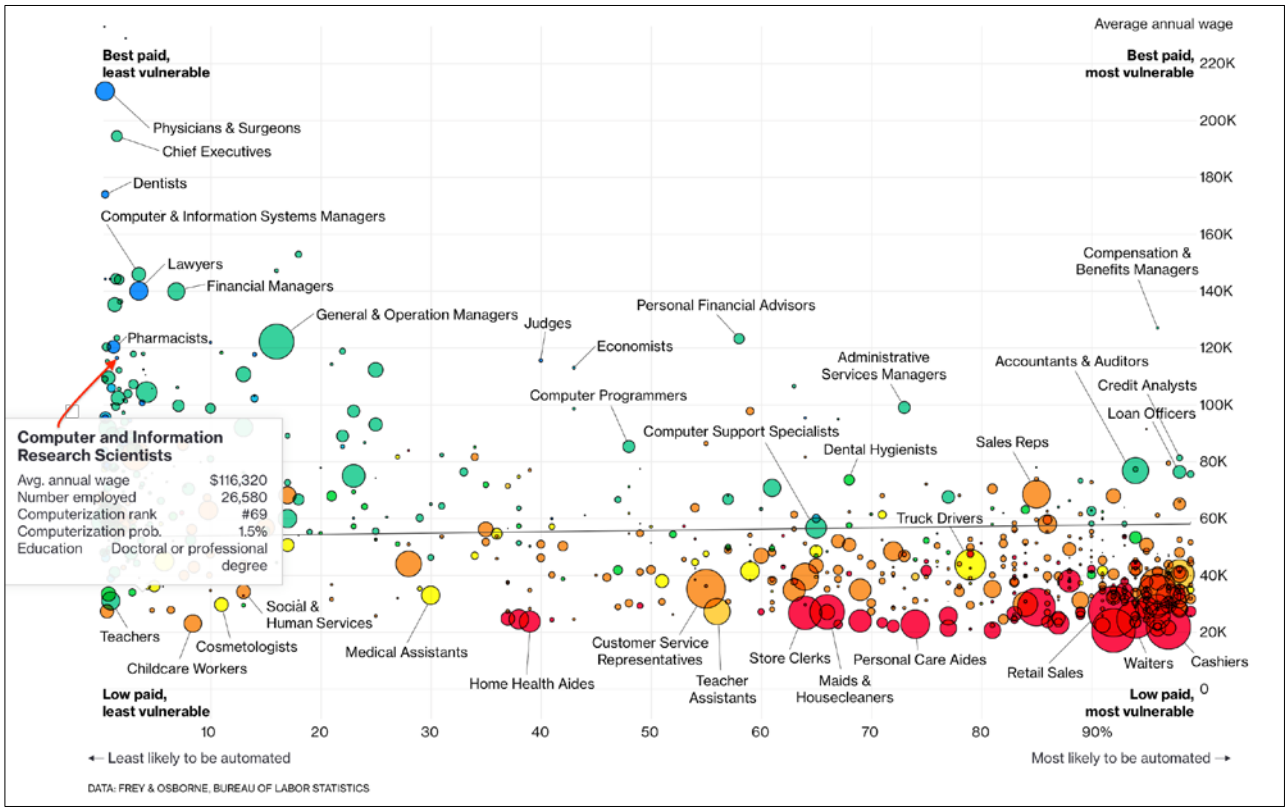
The table below provides a summary of CICAG's planned and proposed future scientific and educational meetings. For more information, please contact CICAG's Chair, Dr Chris Swain (swain@mac.com).

Meeting	Date	Location	Further Information
RSC Historical Collection	2017	Webinars	In partnership with the RSC Library and Historical Chemistry Interest Group
Chemistry on Mobile Devices 2	2018	Burlington House, London	An update of the successful Chemistry on Mobile Devices meeting held in Cambridge in 2016
Spectroscopic Data to Chemical Knowledge	2018	AstraZeneca, Macclesfield	To be organised jointly with the Molecular Spectroscopy Interest Group and Dial-a-Molecule Grand Challenge Network
Faraday Discussion on Big Data and Chemical Information	2018/19	Sheffield or Leeds (approved Faraday Discussion venues)	Faraday Discussions
Celebrate the Centenary of IUPAC	Spring 2019	Burlington House, London	To be organised jointly with the Historical Chemistry Interest Group
Structure, Reaction and Patent Information for Small Organisations	TBD	TBD	Proposed joint meeting with RSC Consulting Group
Software Update for Medicinal Chemists	TBD	EBI, Hinxton, Cambridge	Proposed training workshop (Joint workshop with the SCI)
Big Data	TBD	TBD	Proposed joint meeting with the SCI)

Is Your Job at Risk of being Automated?

With thanks to Mark Whitehouse, Mira Rojanasakul, Paula Dwyer and others at the Bloomberg Newsroom, email pdwyer11@bloomberg.net

Media, publishing and financial information house Bloomberg has recently incorporated a new interactive job automation risk graphic on their site, allowing users to enter an occupation and see the results of calculated risk of the profession becoming automated as robots and artificial intelligence increasingly become capable of undertaking more and more tasks currently performed by humans. Also illustrated are number of US employees and average US salary. Below is the graphic with 'Computer and Research Information Scientists' selected (the nearest category we could find for many CICAG members).



For more information on the data behind the tool and to try it out, visit https://www.bloomberg.com/graphics/2017-job-risk/

International Chemical Identifier for Reactions (RInChI)

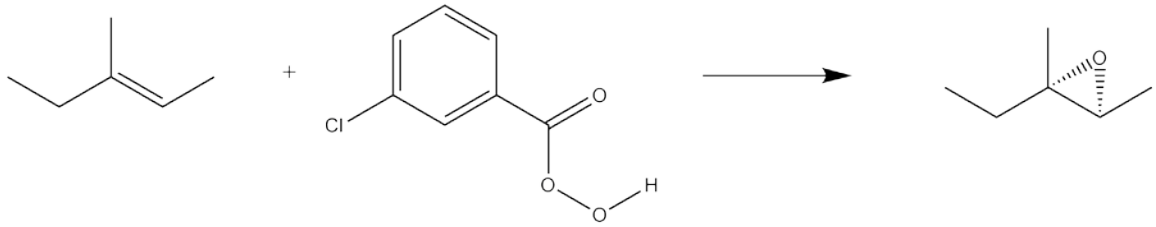
Contributed by RSC CICAG Committee member Professor Jonathan M Goodman, email: jmg11@cam.ac.uk

The *Reaction InChI* (RInChI) is an identifier for reactions,[1] which was developed on similar principles to those used for the InChI identifier.[2] The RInChI provides a concise description of the key data in chemical processes, and facilitates the manipulation and analysis of reaction data. Prototype versions of the RInChI have been available since 2011 and the first official release (RInChI-V1.00), funded by the InChI Trust, is now available for download.[3] The RInChI describes chemical reactions as a unique machine-readable character string, based on the InChI algorithm, and is suitable for data storage and indexing.

It is straightforward to construct a few RInChIs by hand, following the instructions and using the standard InChI generation software. The generation of thousands of RInChIs is much better done using the software available for download from the InChI Trust website.[4] The software also generates RInChIKeys, which are

hashed versions of RInChIs, and auxiliary information which can be helpful in regenerating detailed reaction descriptions. Many examples of RInChIs are available.[5]

RInChI Version 1.00 comprises six layers, which may readily be constructed by hand, provided that a program to generate InChI standard version 1.04 is available. The automated process for doing this will be described in §5.1. The layers are separated by a solidus symbol, commonly called "slash" ("/"), except for the layers which list molecules that are separated by "less than" and "greater than" signs: "<>"

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RInChI=1.00.1S/C6H12/c1-4-6(3)5-2/h4H,5H2,1-3H3/b6-4+!C7H5ClO3/c8-6-3-1-2-5(4-
6)7(9)11-10/h1-4,10H<>C6H12O/c1-4-6(3)5(2)7-6/h5H,4H2,1-3H3/t5-,6-/m0/s1/d+
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RInChIs provide a way of labelling reactions so that different people doing the same reaction should generate the same label. This makes it possible to search large reaction databases quickly, and to discover new insights into chemistry. As more RInChIs become available, the more chemistry we will be able to discover and to understand.

[1] Grethe G, Goodman J M, Allen C. International chemical identifier for reactions (RInChI) *Journal of Cheminformatics 2013*, **5**, 45. DOI: 10.1186/1758-2946-5-45
[2] IUPAC InChI Website: http://www.iupac.org/inchi/ (accessed June 29, 2017)
[3] Download RInChI software: http://www.inchi-trust.org/downloads/ (accessed June 29, 2017)
[4] InChI Trust Website: http://www.inchi-trust.org/ (accessed June 29, 2017)
[5] http://www-rinchi.ch.cam.ac.uk (accessed June 29, 2017)

IUPAC InChI Meeting, August 16-18, NIH

Kindly contributed by Professor Stephen T. Heller, email steve@hellers.com

A three-day meeting, sponsored by the NCBI of the National Library of Medicine (NLM), on the status and future of the IUPAC InChI chemical structure standard will be held at the U.S. National Institutes of Health (NIH) main campus in Bethesda, MD on August 16-18, 2017, just prior to the nearby National American Chemical Society (ACS) meeting in Washington, D.C. (Bethesda is a short Metro/Subway ride from downtown Washington). The meeting will bring together the InChI community, collaborators, working groups, and other interested stakeholders to define and improve upon the current state of the InChI and associated chemical information digital standard projects. A primary aim is to discuss where have come to date, what more is needed for the chemical, biomedical, materials, and related academic and industry communities for proper and useful chemical structure standard representation of both small and large molecules. Setting the future direction and activities of InChI development will be a major goal of the meeting.

The meeting is designed to follow-on from the "Expanding IUPAC Standards for Chemical Information – industry applications & stakeholder perspectives" workshop at the European Bioinformatics Institute (EBI) in Hinxton, U.K. held this past March 2017, this meeting at NIH will include InChI working group sessions and presentations from various stakeholders. The InChI working groups include mixtures (MInChI), tautomers, organometallics, positional isomers, stereochemistry, InChI for reactions (RInChI), QR codes, and the InChI resolver. Presentations about InChI and numerous use cases will be given by speakers from the InChI Trust, chemical publishers, chemical vendors, data vendors, software vendors, pharmaceutical companies, universities, US Government labs and offices, related standards groups and more.

There is no charge to attend the meeting. Registration is available via the InChI Trust web site – www.inchi-trust.org.

Accessing the RSC's Digital Archive

Contribution from John Hudson, Chair of the RSC Historical Group, with input from David Allen (RSC Library) and CICAG Committee Member Dr Helen Cooke

The digitised material in the collection, which is of value to many chemists in addition to those with an interest in historical chemistry, can be accessed and saved by RSC members free of charge. You will need your member username, which is your 6 digit membership number (on your membership card), and your password, which is your date of birth expressed numerically in the format YYYYMMDD.

To Access the Historical Collection

- Go to http://pubs.rsc.org/historical-collection
- On this page there is a panel where you can click to obtain general information on the historical collection and guidance on how to access.

Books and Papers in the Historical Collection

The RSC holds an extensive range of classic works, with titles by Lemery, Lavoisier, Priestley, Davy and others.

- Having reached the Historical Collection page (link above), click on Historical Books and Papers.
- Sign in with your member username and password.
- Either enter a search term, which will search the entire collection, or click on one of the four currently digitised components of the Historical Collection (Main Collection, The Roscoe Collection, Davy Bookcase, or The Nathan Collection), which will bring up a searchable list of the books in that part of the Historical Collection.
- An item in the collection can be downloaded and saved as a PDF file. Not surprisingly, the file sizes for books are large.

Society Publications and Minutes in the Historical Collection

This collection contains material produced by the Royal Society of Chemistry, the Chemical Society and the Royal Institute of Chemistry, including minutes of the Chemical Society from 1841 and the (Royal) Institute of Chemistry from 1877, magazines (e.g. Chemistry in Britain and Education in Chemistry), annual reviews, monographs, and lists of Fellows.
•From the Historical Collection page (link above), click on Society Publications and Minutes.
•Enter a search term (e.g. the title of an article in Chemistry in Britain), or click on one of the components of the collection (e.g. Chemical Society Council Minutes or Chemistry in Britain, and then select year and volume).
•Note: for Chemistry in Britain and Education in Chemistry, when you have selected an issue, only the main articles appear in the contents list. The entire issue can be viewed by clicking the box Download full PDF.

Papers in RSC Journals

Also of great value is the archive of all journals published by the RSC and its predecessor societies from 1841 (with the exception of issues less than 10 years old). This archive is published on a different platform from the Historical Collection, and a different login procedure is required.

- Go to RSC Journals Home.
- Click Log In (top left of screen).
- Here you are offered three login options. Click Log in with your member or subscriber username and password (NOTE this is not the option offered automatically – it is No. 3 on the list).
- Enter your username and password.
- Click Journals.
- In the "Browse by" list, select All Journals (this will list both current and discontinued journals), then enter details in "Find an issue" or "Find an article".
- If you don't have enough details or if you don't have a specific article in mind, try clicking Advanced at top of page, click on Journals, and insert author name and any other available details (e.g. date range).
- Select paper to be viewed by clicking on PDF.
- Download paper.

Philosophical Transactions of the Royal Society

This is not available from the RSC, but go to
Philosophical Transactions of the Royal Society of London Archive

- This gives access to all papers 1665-1886. For papers from 1887 onwards, choose Series A or Series B.
- Select volume and then paper by clicking on PDF.

Proposed Webinars

In collaboration with the Historical Group and the RSC Library, CICAG is intending to run some webinars which will be open to all RSC members, during which users of the Digital Archive will be able to learn more about the collection, and compare their experiences. More information will be made available once details have been finalised. For more information contact Helen Cooke (helen.cooke100@gmail.com).

New CICAG Website

Contributed by RSC CICAG Website Editor Neil Berry, email: ngberry@liverpool.ac.uk

CICAG is pleased to announce the creation of a new website for the group. The site contains information and details concerning the scope and aims of the group, forthcoming events, our twitter feed, archives of previous meetings including presentation slides, current and previous newsletters, details of committee members and key contacts. Having our own dedicated site will allow CICAG to more rapidly add and edit content and disseminate information. We will be looking to expand and enhance the site in the future and so would welcome all suggestions for improvements.

The new website can be found at https://www.liverpool.ac.uk/~ngberry/cicag/index.htm. Please send any feedback directly to myself at the address above.

CICAG Surveys: CICAG Newsletter and Social Media Use

Contributed respectively by Stuart Newbold, RSC CICAG Newsletter Editor, email stuart@psandim.com and Dr Michelle Lynch, RSC CICAG Social Media Editor, email mklchems@gmail.com

Newsletter Survey

Firstly, a new survey to assess views on the CICAG Newsletter and also CICAG meetings and activities is now available. There are six questions. Please take the one or two minutes required to complete the survey and provide us with valuable feedback. We will then share this with members in the winter newsletter and on the new Website (see later article). The survey can be found here:

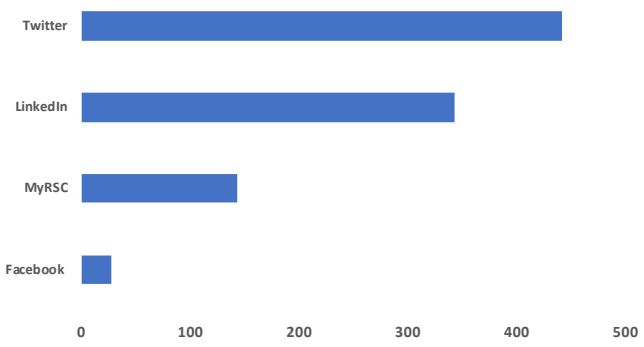
https://www.surveymonkey.co.uk/r/3K6ZVJ2

Recently we also conducted a survey on CICAG membership use of social media, their likes, dislikes and preferences. The results of this exercise are discussed below by Michelle.

Social Media Survey

RSC Chemical Information Computer Applications Group (RSC CICAG) disseminates information through several social media channels as well as through its website and RSC emails. These channels have evolved over time and are mostly used for posting information about RSC CICAG's activities, planned meetings and other activities as well as for posting industry news links and snippets. The membership numbers for each of the social media channels are shown in the chart below. Twitter and LinkedIn are the most popular groups with the largest number of followers, although MyRSC has a significant following and as the survey results will show, is still many members preferred channel. Facebook is the newest channel and is at an early stage of development.

RSC Social Media Channel Membership

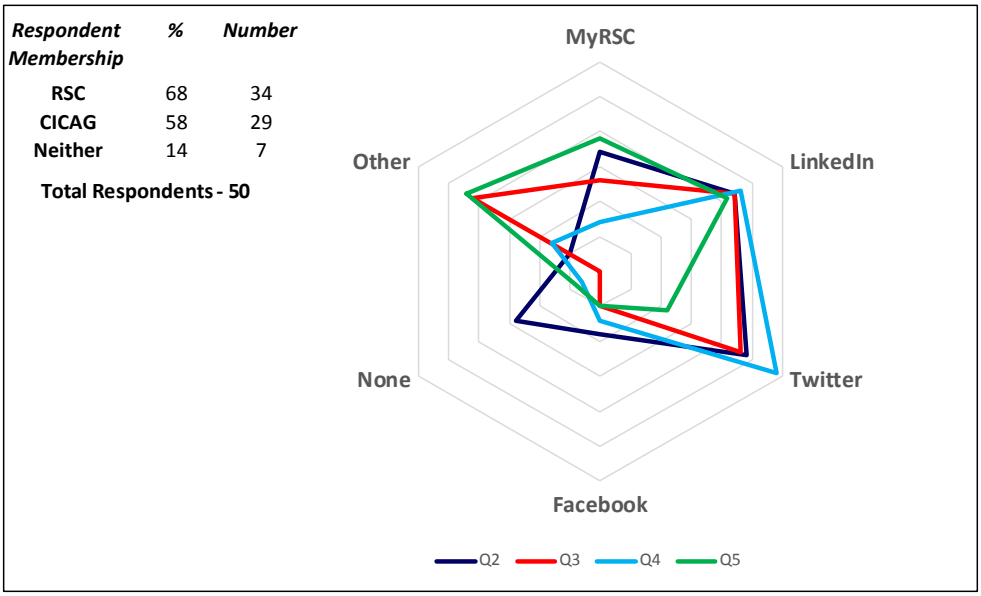


A survey was carried out using the online service Survey Monkey. Respondents were asked a series of 8 questions. The results to the first 5 questions are summarised in the table and radar chart below. Q1 was

simply to establish whether respondents were members of the RSC or the RSC CICAG special interest group. Questions 2-5 were aimed at establishing preferences for receiving different types of content in each channel. The results indicate considerable diversity in people's preferences although the most popular channels for all types of content are Twitter and LinkedIn. Within the 'Other' category, respondents have stated that they like to receive content via the RSC Web Site, RSC emails and RSC Update magazine, in particular for finding out about CICAG organised meetings. The most popular channel (58% of responses) for receiving news snippets is Twitter and second most popular (44% of responses) is LinkedIn. There was a spread of preferences for being alerted to the publication of RSC CICAG meeting reports and newsletters. LinkedIn and MyRSC were the most important channels followed by a range of 'Other' methods including Email and Web Site.

RSC Social Media Survey Results

Social Media Channel	*Q2. Do you use any of the following RSC CICAG social media channels*		*Q3. Where would you prefer to find out about CICAG organised meetings?*		*Q4. Where would you prefer to see relevant news snippets?*		*Q5. Where would you prefer to go to find RSC CICAG meeting reports, newsletters etc.?*	
MyRSC	34%	17	26%	13	14%	7	38%	19
LinkedIn	44%	22	44%	23	46%	23	42%	21
Twitter	48%	24	46%	22	58%	29	22%	11
Facebook	18%	9	10%	5	14%	7	10%	5
None	28%	14	0%	0	6%	3	8%	4
Other	10%	5	42%	21	16%	8	44%	22



Questions 6-8 gave people the opportunity to provide open feedback regarding RSC CICAG's use of social media.

Question 6: RSC CICAG's Social Media is most useful to me for:
Replies to this question indicate that announcements of RSC CICAG and related interest group meetings, reports and newsletters were regarded as the most useful Social Media content.

Question 7: If I could improve one thing about RSC CICAG's Social Media it would be:
Most responses requested a focus on RSC CICAG's core activities, meetings, initiatives, video content, virtual conference coverage and links to slide decks. Some people had never used any of the Social Media channels and were surprised to find out about them. Regarding news snippets, responses were polarised between people really appreciating a regular service and those not wanting it at all.

Question 8: Do you have any other comments?

Several respondents like the way that the Social Media channels have evolved and encouraged continuation of our efforts in this area. One or two have asked us not to forget "traditional methods" and believe that we should publicise meetings and events first through emails to members, rather than hearing about them through a Social Media channel open to a wider audience. Similar comments listed in response to Question 7 were provided in answer to this question.

We would like to thank everyone who took part in the survey. The results have provided much food for thought. Clearly Social Media is very important to our members and each individual has a different set of needs to be catered for. We will be giving further consideration how to use each of our Social Media channels taking into account the feedback we've received from you. Clearly there are some very strong preferences for focussing on RSC CICAG content in terms of meetings, news and publications. Many of you also find news snippets and relevant discussions helpful too. Members of the RSC, RSC CICAG and the wider chemicals community are all invited and encouraged to participate in our Social Media activities by following and tagging us on Twitter, posting on Linkedin, joining/viewing our Facebook and MyRSC groups. A reminder of where to find us is given below.

Twitter: https://twitter.com/RSC_CICAG/
Linkedin: https://www.linkedin.com/groups/1989945
Facebook: https://www.facebook.com/groups/RSCCICAG/
MyRSC: http://my.rsc.org/groups/home/546
Web Sites: http://www.rsc.org/Membership/Networking/InterestGroups/CICAG/ and
https://www.liverpool.ac.uk/~ngberry/cicag/index.htm

Catalyst Science Discovery Centre and Museum Crowdfunding Project

By RSC CICAG Treasurer Dr Diana Leitch MBE, email diana.leitch@googlemail.com.

Dear Fellow CICAG Members. Several of you know that as well as my role as CICAG Treasurer I am a Trustee at the Catalyst Science Discovery Centre and Museum (www.catalyst.org.uk) in Widnes, Cheshire, which is the only Science Discovery Centre in the UK which is focussed on promoting the chemical sciences to people of all ages but particularly young people. This year Catalyst is celebrating 30 years of educational provision since 1987 when it was founded as a Museum to celebrate the glorious past of the area of Runcorn and Widnes which had been the great heartland of the chemical industry. This is mine and my family's background going back for over 200 years. Catalyst's current slogan is 'Preserving the Past and Promoting the Future'. We are also very keen in an area with horrendous unemployment (49% around our building) to encourage local young people to believe they can have a future and can also go on to succeed in chemical sciences and STEM. We have several local scientific heroes born in Runcorn or Widnes, as I was and they were, who can be eminent role models for these young people and we are keen to showcase some of these people.

Last year we applied to two funding bodies to create a new gallery celebrating the tremendous work of four members of the Baker family born and brought up in Runcorn, who went on to succeed at national and international level in chemistry, mechanical engineering and botany. The chemists, Dr Harry Baker (student of Bunsen and Henry Roscoe and first Works Chemist at the ICI Castner Kellner Works) and his son, Professor Wilson Baker FRS, through their work on chlorine and synthetic penicillin, can be said to have saved millions of lives worldwide. They were members of the RSC for 121 years continuously from 1881 to 2002. Professor Wright Baker FEng, Professor of Mechanical Engineering at UMIST, opened the Dead Sea Scrolls from Qumran, and his wife Dr Kathleen Drew Baker, a dedicated botanist, saved the Nori Seaweed industry in Japan where she is revered. All were graduates of Owens College/University of Manchester, and were Quakers. Wilson Baker founded Oxfam. The funding application was described as very strong, designs had been done, but it was disappointingly not funded. Undeterred we have just launched a Crowdfunding

Project to try to fund this gallery in a different way. We have until 25 August under Crowdfunding rules to try to raise the £40,000 we need to create the gallery. Any publicity you can assist with by any forms of media or small amounts of money that can be pledged would be most welcome.

The Crowdfunding site is www.crowdfunder.co.uk/harry-baker-and-his-amazing-familys-achievements

Dr Diana M. Leitch MBE, BSc, PhD, FRSC

Treasurer, RSC-CICAG, and Trustee at Catalyst Science Discovery Centre and Museum

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Undergraduate Research Bursaries – CICAG Sponsorship in 2018

Contributed by RSC CICAG Committee Member Neil Berry, email: ngberry@liverpool.ac.uk

A number of Undergraduate Research Bursaries, funded by the Royal Society of Chemistry, are available each year to students in UK and ROI Chemistry and related departments to fund research projects which this year run from June-September 2017. The purpose of the awards is to give experience of research to undergraduates with research potential in the middle years (i.e. 2/3, 2/4 or 3/4) of their degree and to encourage them to consider a career in scientific research. CICAG agreed to sponsor one student project. We are pleased to report that the recipient will be Grzegorz Winter, who is studying at Newcastle University and his project will be the School of Chemistry. The title of his project is "Re-writing the functional form of classical force fields for molecular simulations".

Further information, including guidelines, the application form and deadlines, can be found at http://www.rsc.org/ScienceAndTechnology/Funding/undergraduate-bursary.asp

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Chemical Information / Cheminformatics and Related Books

Contributed by RSC CICAG Newsletter Editor Stuart Newbold, email: stuart@psandim.com

Elsevier Analytical Services has recently published "*World of Research – The Global Research Landscape at a Glance*". The book is available as a free PDF download and provides a snapshot of essential research indicators for the most prolific countries or regions in the world. It contains 77 national profiles and comprises general statistics and graphs along with analyses and interpretations.

Tony Kent Strix Award and Annual Lecture 2017

Contributed by RSC CICAG Member Dr Doug Veal, email dougveal@waitrose.com

UKeiG - 2017 Call for Tony Kent Strix Award Nominations

The UK electronic information Group (UKeiG) is now seeking 2017 nominations for this prestigious award. The Tony Kent Strix Award is given in recognition of an outstanding practical innovation or achievement in the field of information retrieval in its widest sense, including search and data mining, for example. This could take the form of an application or service, or an overall appreciation of past achievements from which

significant advances have emanated. The award is open to individuals or groups from anywhere in the world.

The deadline for nominations is Thursday 31st August 2017.

Nominations should be for achievement that meets one or more of the following criteria:

- A major and/or sustained contribution to the theoretical or experimental understanding of the information retrieval process
- Development of, or significant improvement in, mechanisms, a product or service for the retrieval of information, either generally or in a specialised field
- Development of, or significant improvement in, easy access to an information service
- Development and/or exploitation of new technologies to enhance information retrieval
- A sustained contribution over a period of years to the field of information retrieval for example, by running an information service or by contributing at national or international level to organisations active in the field.

Key characteristics that the judges will look for in nominations are innovation, initiative, originality and practicality.

The information to be supplied in the nomination should comprise:

- The name, institutional address and qualifications of the nominee
- A brief biography (not more than one page of A4)
- A relevant bibliography (i.e. not comprehensive but including the key publications relevant to the nomination)
- A justification for the nomination, of not more than one page of A4, showing clearly which of the Strix award criteria the nominee meets and how the criteria are met
- Additional material (e.g. letters of support - letters from past winners would be especially valuable).

It is possible that the Award Committee will request additional information from the nominators for those nominees considered suitable candidates for the award.

Nominations for the 2017 award should reach the judges by Thursday August 31st 2017 and be emailed to:

John Wickenden – Hon. Secretary UKeiG secretary.ukeig@cilip.org.uk
cc-ed to Gary Horrocks - UKeiG administrator admin@ukeig.org.uk
cc-ed to Sue Silcocks – Hon. Treasurer UKeiG treasurer.ukeig@cilip.org.uk

UKeiG presents the Tony Kent Strix Award in partnership with the International Society for Knowledge Organisation (ISKO UK) and the British Computer Society Information Retrieval Specialist Group (BCS IRSG). The award is sponsored by the Royal Society of Chemistry Chemical Information & Computer Applications Group.
For further information please visit the Awards & Bursaries section of the UKeiG web site: www.ukeig.org.uk/.
UKeiG is a Special Interest Group of CILIP, Registered Charity Number 313014.

Meeting Report: RSC Annual General Meeting

By RSC CICAG Treasurer Dr Diana Leitch MBE, email diana.leitch@googlemail.com.

I attended the AGM of the Royal Society of Chemistry at Burlington House on Wednesday, 12th July, in order to hear about the new strategy of the RSC, to network with members of their senior staff, several of whom are fairly new to the RSC, and to meet new members of Council. A full report of the meeting will

appear subsequently in Chemistry World and the newly renamed Voice (replacement for RSC News) so this is a short report.

The meeting was chaired by Sir John Holman, the current President, and the financial report was given by the outgoing Treasurer, David Grayson. The meeting was quorate with 20 members present. The immediate Past President, Professor Dominic Tildesley, was thanked for all his work and the incoming President-Elect, Dame Carol Robinson (University of Oxford), was welcomed. She becomes President in July 2018. She started as a Graduate trainee, worked in the pharmaceutical industry and is a winner of the Rosalind Franklin Award.

The President reviewed the strategy of the last period which had 5 strategic priorities – promotion of the chemical sciences, encouragement of skills development, provision of chemical knowledge, support of membership, and development of organisational strength. Some highlights of these were the endless discussions about Brexit and its effects, meetings with Minister Jo Johnson and attendance at 15 government consultations, the support of 50 Outreach projects including Tim Peake and space, the support of emerging technologies, providing a well-trained supply of professional chemists – 15,000 CChems, 15 Registered Scientists and 15 Registered Technicians (he wished there were more of the latter). Other highlights were his influence on education policy as he is passionate about education and he has been giving evidence to the House of Commons (England) review, the production of 42, 000 journal articles, 100 new book titles, the move to Open Access by the publishing group, and organisation of 200 conferences and events around the world. The membership was praised for their giving of 'Time for Chemistry'. In terms of strengthening the organisational structure, the budget was much healthier than it had been and the deficit budget set for 2016 of £6 million had not had to be invoked because overall savings prevented this from happening and the governance review had been started.

The strategy for the next 5 years (2017-2020) encompasses the following 3 core roles for the RSC

a) To be a provider of high-quality chemical sciences knowledge to all who need it

b) To be the UK's professional society for chemists – monitoring standards, supporting development and covering a wide-range of professions in chemistry

c) To defending chemistry and to speak in the best interests of chemistry so as to influence decision makers; ensuring chemistry has a Voice

RSC members are needed to support every aspect of the strategy.

There will be a Governance Review during the next year and the results will be presented at the 2018 AGM.

Preparations are going ahead for a celebration with the German Chemical Society of their 150th Anniversary this year.

Meeting Report: Chemical Structure Representation – What Would Dalton Do Now?

By RSC CICAG meeting organising committee member, Dr Helen Cooke, email: helen.cooke100@gmail.com

This meeting, held at Liverpool University on 22 June 2017, explored current and future problems with structure representation, possible solutions and innovations necessary to overcome them. There was a strong focus on challenging structures and the limits of molecular representation, e.g. materials, biologicals and polymers, the feeling being that solutions for small organic molecules were already well established. The morning session was mainly concerned with identifying the problem areas; the afternoon primarily discussed possible ways forward and solutions.

Above: Panel discussion at the afternoon session

There was a broad diversity of attendees, the majority of whom were from industry. A number were from organisations based in the North West, which we were pleased to see as in 2016 and 2017 we have been widening our outreach by organising events outside London.

CICAG was pleased to have been able to sponsor a student bursary which was awarded to Gianmarco Ghiadoni, PhD student in Professor Peter Willett's group in the Information School at the University of Sheffield.
At lunch time there was an interesting tour of Liverpool University's award-winning Central Teaching Hub, which consolidates much of the undergraduate teaching within the Faculty of Science and Engineering. https://www.liverpool.ac.uk/central-teaching-hub/

Some themes and observations I noted were:

- Setting standards is at the heart of international exchange of information and IUPAC has played a crucial role.
- How structures are represented has varied over time, and sometimes even within the same paper.
- Looking at molecules from different angles can simplify understanding.
- Merging data and information acquired via different structure determination techniques helps to build a more comprehensive picture.
- Large molecules, such as proteins, are not compatible with all-atom representations.
- Tautomerism, organometallics and multicomponent systems are still a big problem.
- There are at least 63 ways of representing a nitro group!
- Natural language processing will soon be good enough to enable computers to read with human-like understanding.
- Peer review: in the future machines will tell us what's new in a paper, what's repeating work reported elsewhere, and even when your work contradicts that of others.
- The community needs to pull together – problems still exist, for example, with mixtures, chirality, large molecules.
- Dialects of established representation notations/languages are evolving to accommodate different kinds of structures.
- Representing inorganic compounds and materials is increasingly important, with ratios and compositions often more important than connectivity.
- Merging data from different sources or organisations is a challenge.

Several speakers drew attention to an upcoming meeting "State and Future of the IUPAC InChI" at the NIH 16-18 August 2017, and delegates were encouraged to attend. See http://www.inchi-trust.org/ and the separate article in this Newsletter for more information.

There was a good Twitter discussion during the meeting (search #CICAGDalton to see all Tweets), the themes and discussion points are represented in the word cloud below, produced by Neil Berry.

The presentations were as follows:

- IUPAC: the role of international organisations in nomenclature and terminology in the internet age. Professor Jeremy Frey, Department of Chemistry, University of Southampton
- Indescribable structure: finding words for the future. Professor Jonathan Goodman, Department of Chemistry, University of Cambridge
- Biology: bigger models, bigger confusion. Dr David C Briggs, Department of Life Sciences, Imperial College London
- Chemical structure representation challenges encountered when curating the CSD. Dr Matt Lightfoot, Editor in Chief, Cambridge Structural Database, CCDC
- Keynote: Describing chemical substances and chemical structures: we have a long way to go. Dr Evan Bolton, Chemistry Program Head, US National Center for Biotechnology Information (NCBI)
- Using data science techniques to put molecules in context. Dr Aileen Day, Data Scientist, Royal Society of Chemistry
- Chemical structure representation of inorganic salts and mixtures of gases: A newer system of chemical philosophy. Dr Roger Sayle, CEO and Founder, NextMove Software Ltd
- Extracting medicinal chemistry knowledge by a secure Matched Molecular Pair Analysis Platform: standardization of SMIRKS enables knowledge exchange. Dr Al Dossetter, Managing Director, MedChemica Ltd
- InChIs are part of the solution. Mr Richard Kidd, Publisher, Royal Society of Chemistry and Treasurer, InChI Trust
- HELM: Setting the standard for biomolecular information exchange. Claire Bellamy, HELM Project & CSCS Expert Community Manager, Pistoia Alliance

The presentation slides, speakers' abstracts and biographies are available on the meeting web page http://www.rsc.org/events/detail/23638/chemical-structure-representation-what-would-dalton-do-now

We are grateful to the CSA Trust for providing funding for our keynote speaker, Evan Bolton, to travel from the USA to attend the meeting.

CICAG Accounts are Available on Request

Contributed by RSC CICAG Newsletter Editor Stuart Newbold, email: stuart@psandim.com

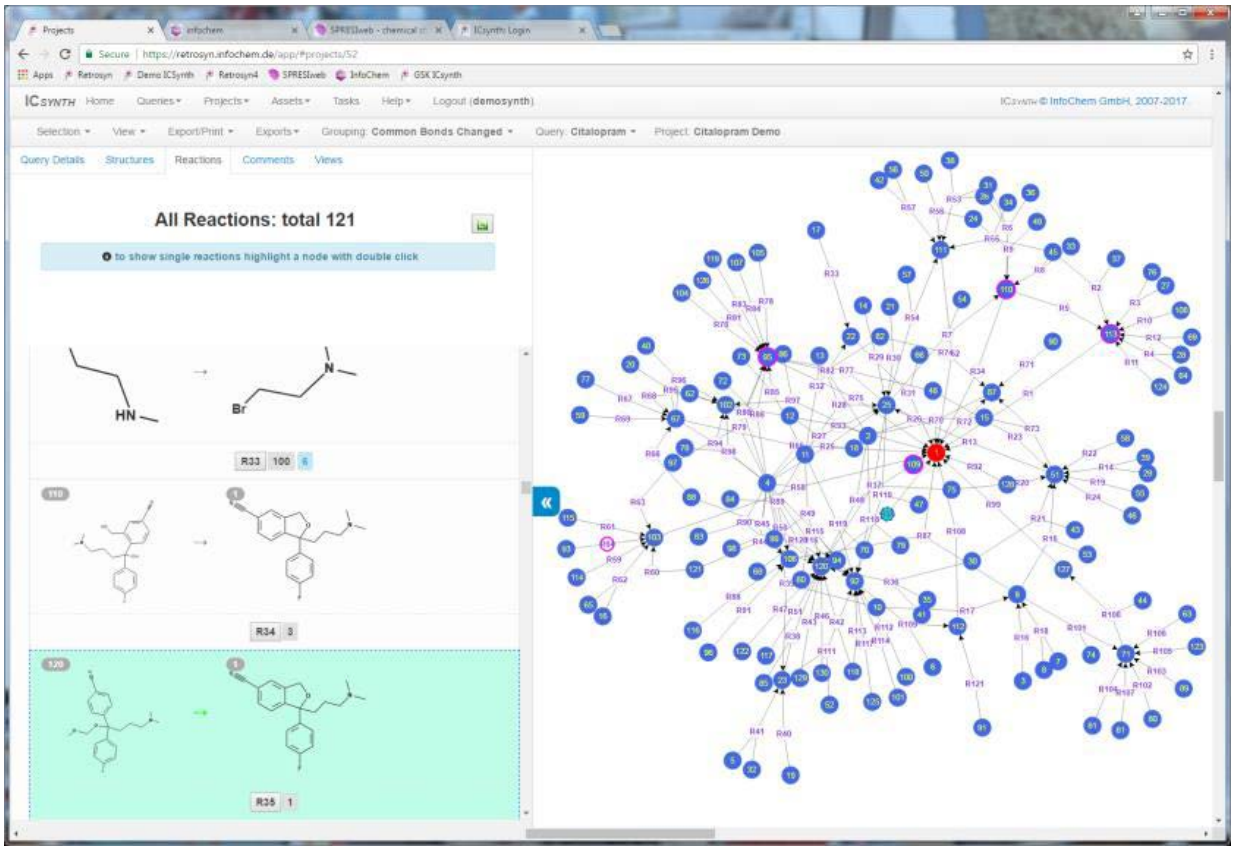
The group is extremely grateful to CICAG Treasurer Dr Diana Leitch MBE for her continued service in this valuable role. Please note that CICAG annual accounts are available to all members who request a copy. If you as a member would like to receive a copy, please contact Diana on diana.leitch@googlemail.com.

InfoChem News

Contribution from Dr Valentina Eigner-Pitto, email: ve@infochem.de

ICSYNTH Version 3.0 Launched

InfoChem is pleased to announce the release of ICSYNTH version 3.0 in Q2 2017. ICSYNTH is a powerful synthesis-planning tool able to define synthesis routes based only on fully algorithmic chemical knowledge and not on literature based synthesis path analysis. The system builds multistep, interactive synthesis trees taking advantage of automatically created transform libraries derived from literature and patent reaction data. The user is able to interact with the software selecting different synthesis strategies and defining the number of precursors and steps.
A significant advantage of ICSYNTHs concept is the possibility of generating rapidly and straightforwardly in-house libraries of transforms based on companies' proprietary and confidential reaction data (e.g. ELNs), for private use in their own ICSYNTH installations.



Two major enhancements characterize version 3.0 of ICSYNTH. First, the reaction layout view introduced with V.2.2 has been enhanced to become a genuine reaction graph: precursors can be visualized as molecules or just kept as nodes. The side panel enables magnification of the information in the graph, giving users an immediate scan of the highlighted reaction, empowering easy browsing of the retrosynthetic analysis results. The second major improvement provides the possibility to work in a team. ICSYNTH V.3.0 enables project managers to define user groups able to work on the same target molecule, adding comments and exchanging information directly in the web-application. Furthermore the algorithm responsible for the precursor search has been improved, resulting in better pathway suggestions.

For more information about ICSYNTH, please visit our homepage (http://www.nature.com/content/infochem/icsynth/index.html) or contact us (info@infochem.de).

CAS / SciFinder / STN News

Contributed by CAS Applications Specialist in the UK & Ireland, Dr Anne Jones, email annejones@acs-i.org.

Meet Your New Lab Partner! Introducing SciFinder^n

Do exponentially more. SciFinder^n will get you on your way and back to the bench faster than any other solution. At least that's what users are already telling us!

Our research shows that scientists have to spend a lot of time perfecting queries and reviewing results. With the all-new SciFinder^n you will get valuable, high-quality information in a new easy-to-use interface of course, but more importantly you will get real insights from fellow scientists at CAS and time saved.

Researchers will find SciFinder^n offers confidence and trust in the easiest-to-use solution on their device of choice. Information professionals and management will find SciFinder^n is the best value for their investment.

- Reduces result set review time with significant advances in query/search relevancy
- Offers more content than any SciFinder® product - ever. Includes easy access to full-text, indexed patents, and millions of step-by-step syntheses indexed specifically by CAS
- Powerful, easy-to-use interface that helps you at every step
- Expanded access for your entire organization as well as new product administration features

CAS and Wiley Announce ChemPlannerTM Collaboration

CAS and John Wiley & Sons have announced a collaboration that will enhance the ChemPlanner predictive synthesis tool with CAS reaction content and integrate it into SciFinder^n as an exclusive distribution channel. Through this partnership, CAS is taking a leadership role in advancing predictive synthesis technology, consistent with our strategic vision to be an innovative information solutions provider by increasing sophistication of our solutions to solve market problems more effectively.

ChemPlanner is a system that helps chemists design viable synthetic routes to their target molecules by suggesting alternative synthetic strategies, and exposing a spectrum of relevant synthetic methods and available building blocks. The system derives its knowledge from reaction databases and carries out retrosynthetic analysis from the target back to commercially available starting materials.

- Synthetic paths combine published and predicted reaction steps to synthesize targets for which no current synthetic path is known
- Used for challenging new molecule syntheses and also to optimize known processes
- Includes content from Wiley's CIRX (Cheminform) reaction database

STN News

There is now a better way to access the full power and value of classic STN®.

Introducing STNext™, a new gateway to the world's premier solution for scientific, technical and IP research!

Built on the classic STN foundation and available to you now at no additional charge*, STNext delivers the comfort and confidence of STN in a new, browser-based interface:

Securely access STN from any computer, without the hassle of desktop software or plug-ins
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Take immediate advantage of the latest STN enhancements

For a limited time, there is free access to PatentPak® exclusively on STNext. Take this opportunity to see how you can leverage the work of CAS scientists to radically reduce the time you spend acquiring patents and pinpointing the relevant chemical substance information within them.

New STN

The April 10 release of new STN® delivered highly requested improvements for search histories with a new, more compact format and the ability to select individual queries (i.e., L-numbers), enabling users to customize content and speed review of prior search activity.

Other highlights of the release include:

- Addition of two databases, Chemical Business NewsBase (CBNB) and the Rapra Polymer Library (RAPRA), expanding our coverage of business news and non-patent literature for plastics, rubber and polymers
- Legal status information from 77 patent authorities is now available in INPADOC
- All new STN databases can now be exported to Microsoft Excel® and XML, giving users the flexibility to efficiently export search results in the format that best fits their workflow and search environment

CAS Training in the UK 2017

In addition to the e-learning materials, CAS continues to offer instructor-led training for STN, SciFinder, NCI Global, ChemZentTM, PatentPakTM and MethodsNow in the UK. We conduct 'in-house' or WebEx training sessions on all aspects of searching CAS solutions.

If you wish to know more about any of the CAS solutions or would like further information or help, then please contact annejones@acs-i.org

Anne Jones
CAS Applications Specialist UK & Ireland

Other Chemical Information Related News

With a special thanks to RSC CICAG Member Dr Keith White

Milk versus dark chocolate: A scientific showdown (video)
Which variety is the better choice: milk or dark chocolate? '*Reactions*' pits the two against each other in a scientific showdown, highlighting research on chocolate's potential health benefits, flavour, aphrodisiac properties and more. Check out this confectionary competition here:
https://www.youtube.com/watch?v=8rSaOv8vZyY.
Source: ACS (contact ACS Newsroom newsroom@acs.org)

Google acquires data science community Kaggle
https://techcrunch.com/2017/03/07/google-is-acquiring-data-science-community-kaggle/
Source: TechCrunch

How GSK works with Yammer
Does your organisation make use of Yammer as an information sharing and discussion tool? See how GSK adopted the technology; including appointing "Yambassadors" (there is a video at the end of the piece).
https://www.linkedin.com/pulse/how-gsk-works-yammer-janus-boye
Source: Janus Boye

Database of hazardous reactions launched
http://cen.acs.org/articles/95/i12/Database-hazardous-reactions-launched.html
Source: Chemical & Engineering News, March 20, 2017 Issue - Vol. 95 Issue 12

Innovative new features at ScienceOpen
http://www.stm-publishing.com/innovative-new-features-at-scienceopen/
Source: STM Publishing News

The challenges of moving between academia and industry
Chemjobber, http://chemjobber.blogspot.co.uk/ on the challenges of moving from industry to academia—and vice versa
http://cen.acs.org/articles/95/i12/challenges-moving-between-academia-industry.html
Source: Chemical & Engineering News, March 20, 2017 Issue - Vol. 95 Issue 12

University of Houston physicist launches new journal for materials science
https://www.eurekalert.org/pub_releases/2017-03/uoh-upl031517.php
Source: EurekAlert!

Wishes Can Come True: The ChemDraw Innovation Challenge Starts Now!
If ever you have an idea for an improvement in the ChemDraw drawing package…
http://blog.cambridgesoft.com/post/2017/03/14/wishes-can-come-true-the-chemdraw-innovation-challenge-starts-now.aspx
Source: PerkinElmer

LabNetwork Integrates with Reaxys to Offer Seamless Experience from Chemistry Research to Purchase
LabNetwork's nearly four million commercially available discovery and research compounds will now be directly available to users of Reaxys.
http://www.prnewswire.com/news-releases/labnetwork-integrates-with-reaxys-to-offer-seamless-experience-from-chemistry-research-to-purchase-300429433.html
Source: Cision PR Newswire

Turning to Chemistry for New "Computing" Concepts
http://www.darpa.mil/news-events/2017-03-23
Source: Defense Advanced Research Projects Agency

How old are the chemical societies in Australia, Germany, Japan, UK, and USA?
http://www.chemistryviews.org/details/news/10314061/How_old_are_the_chemical_societies_in_Australia_Germany_Japan_UK_and_USA.html
Source: ChemistryViews

It's not just you: science papers are getting harder to read
Modern scientific texts are more impenetrable than they were over a century ago, suggests a team of researchers in Sweden
http://www.nature.com/news/it-s-not-just-you-science-papers-are-getting-harder-to-read-1.21751
Souce: Nature News & Comment

Major internet providers say will not sell customer browsing histories
http://www.reuters.com/article/us-usa-fcc-data-idUSKBN1722D6
Source: Reuters

Start-up showcases organic chemistry education app
http://acsmeetings.cenmag.org/start-up-showcases-organic-chemistry-education-app/
Source: C&EN; ACS Meetings

Cambridge University Press partners with AJE to launch new language editing service for authors
http://www.cambridge.org/about-us/media/press-releases/cambridge-university-press-partners-aje-launch-new-language-editing-service-authors
Source: Cambridge University Press

How Referencing Can Impact Reproducibility
References are more important than most researchers realis and can greatly influence the reproducibility of research work.
http://www.advancedsciencenews.com/references-can-impact-reproducibility/
Source: Advanced Science News

Chemistry and computer coding brought together in NSF-funded institute
http://acsmeetings.cenmag.org/chemistry-and-computer-coding-brought-together-in-nsf-funded-institute/
Source: C&EN; ACS Meetings

Harnessing the power of peer review: Taylor & Francis announce new trial with Publons
http://newsroom.taylorandfrancisgroup.com/news/press-release/harnessing-the-power-of-peer-review-taylor-francis-announce-new-trial-with
Source: Informa/T&F

Fake news and the librarian's duty of care
http://www.infotoday.eu/Articles/Editorial/Featured-Articles/Fake-news-and-the-librarians-duty-of-care-117248.aspx
Source: Information Today

Google uses neural networks to translate without transcribing
https://www.newscientist.com/article/2126738-google-uses-neural-networks-to-translate-without-transcribing/
Source: New Scientist

Why open source pharma is the path to both cheaper and new medicines
https://www.theguardian.com/commentisfree/2017/apr/19/why-open-source-pharma-is-the-path-to-both-cheaper-and-new-medicines
Source: The Guardian

Picture perfect: Cartoon abstracts are a very effective way to bring research to life
https://www.researchinformation.info/feature/picture-perfect
Source: Research Information

Wolters Kluwer Announces Strategic Alliance with Intellectual Property Service Provider ktMINE
http://wolterskluwer.com/company/newsroom/news/2017/04/wolters-kluwer-announces-strategic-alliance-with-intellectual-property-service-provider-ktmine.html
Source: Wolters Kluwer Legal & Regulatory

British Library announces partnership to extend its iconic London building
https://www.bl.uk/press-releases/2017/april/st-pancras-transformed-development-partner
Source: The British Library

Most Innovative Universities - 2017 / Top 100 European Innovative Universities Comparison

http://www.reuters.com/article/us-reutersrankings-europeanuniversities-idUSKBN17Z09T
Source: Reuters

Using PyMOL as a Platform for Computational Drug Design
http://www.advancedsciencenews.com/using-pymol-platform-computational-drug-design/
Source: Advanced Science News

ProQuest and InfoReady Simplify Grant Workflow
http://www.proquest.com/about/news/2017/ProQuest-and-InfoReady-Simplify-Grant-Workflow.html
Source: Proquest

Science publishers try new tack to combat unauthorized paper sharing
http://www.nature.com/news/science-publishers-try-new-tack-to-combat-unauthorized-paper-sharing-1.21959
Source: Nature News & Comment

Brainstorming is not the way to discuss scientific issues
http://www.nature.com/news/brainstorming-is-not-the-way-to-discuss-scientific-issues-1.21951
Source: Nature News & Comment

SwRI turbocharges drug discovery using mobile phone technology
https://globenewswire.com/news-release/2017/05/16/986654/0/en/SwRI-turbocharges-drug-discovery-using-mobile-phone-technology.html
Source: Global Newswire

Derwent Innovation is new name for Thomson Innovation, reflecting proud heritage
http://news.clarivate.com/2017-05-23-Derwent-Innovation-is-new-name-for-Thomson-Innovation-reflecting-proud-heritage
Source: Clarivate Analytics

Copyright Clearance Center Broadens Access to Full-Text Semantic Search with New RightFind® XML for Mining Features
http://www.copyright.com/copyright-clearance-center-broadens-access-full-text-semantic-search-new-rightfind-xml-mining-features/
Source: Copyright Clearance Center

Pay-to-view blacklist of predatory journals set to launch
http://www.nature.com/news/pay-to-view-blacklist-of-predatory-journals-set-to-launch-1.22090
Source: Nature News & Comment

Clarivate Analytics acquires market leader Publons, creating the definitive publisher-independent platform for accelerating research through peer review
http://news.clarivate.com/2017-06-01-Clarivate-Analytics-acquires-market-leader-Publons-creating-the-definitive-publisher-independent-platform-for-accelerating-research-through-peer-review
Source: Clarivate Analytics

IOP Publishing launches RemarqT pilot on a number of journals
Remarq is a new tool for the publishing community which allows annotation, commenting, article sharing, and collaboration, all on the publisher's site.
https://redlink.com/iop-publishing-launches-remarq/
Source: RedLink

Prediction of Organic Reaction Outcomes Using Machine Learning
http://pubs.acs.org/doi/full/10.1021/acscentsci.7b00064
Source: ACS Central Science (ACS Publications)

Elsevier Launches New Reaxys Medicinal Chemistry to Facilitate Better Connections Between Biological and Chemical Data

New search functionality now incorporates machine learning algorithms.
http://www.prnewswire.co.uk/news-releases/elsevier-launches-new-reaxys-medicinal-chemistry-to-facilitate-better-connections-between-biological-626750731.html
Source: Cision PR Newswire

Text-mining tool seeks out 'hidden data'
http://www.nature.com/news/text-mining-tool-seeks-out-hidden-data-1.22132?WT.ec_id=NEWSDAILY-20170609
Source: Nature News & Comment

Online tool connects drug industry to U.K. academia
http://cen.acs.org/articles/95/i24/Online-tool-connects-drug-industry.html
Source: Chemical & Engineering News, June 12, 2017 Issue - Vol. 95 Issue 24

How Cloud Computing Can Shape the Pharmaceutical Industry
https://www.scientificcomputing.com/article/2017/06/how-cloud-computing-can-shape-pharmaceutical-industry
Source: Scientific Computing

Flash card app for chemistry gamifies learning
https://www.elsevier.com/connect/flash-card-app-for-chemistry-gamifies-learning
Source: Elsevier

World's most influential journals for 2017 unveiled in the Journal Citation Reports from Clarivate Analytics
http://news.clarivate.com/2017-06-14-Worlds-most-influential-journals-for-2017-unveiled-in-the-Journal-Citation-Reports-from-Clarivate-Analytics
Source: Clarivate Analytics

Python-Based Software for Computational Drug Design
http://www.advancedsciencenews.com/python-based-software-computational-drug-design/
Source: Advanced Science News

Elsevier and SolveBio announce collaboration to accelerate precision medicine research
https://www.scientific-computing.com/news/elsevier-and-solvebio-announce-collaboration-accelerate-precision-medicine-research
Source: Scientific Computing World

Elsevier launches new version of PharmaPendium
The solution has a number of improvements, to accelerate drug discovery through the comprehensive prediction and assessment of drug-drug interactions.
https://www.elsevier.com/about/press-releases/science-and-technology/elsevier-launches-solution-to-accelerate-drug-discovery-through-comprehensive-prediction-and-assessment-of-drug-drug-interactions
Source: Elsevier

Making research more discoverable: improved functionality on Taylor & Francis Online
http://newsroom.taylorandfrancisgroup.com/news/press-release/making-research-more-discoverable-improved-functionality-on-taylor-francis
Source: Informa/T&F

Big pharma turns to AI to speed drug discovery, GSK signs deal
http://uk.mobile.reuters.com/article/technologyNews/idUSKBN19N003
Source: Reuters
